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Abstract / Kurzfassung

This report describes the numerical CASINOCO - code for the calculation of the surface impedance of normal conducting materials at arbitrary temperatures and arbitrary frequencies up to the infrared region. The code is based on a physical model which considers contributions of nonlocal and retarded current - field correlations.Therefore the universal surface impedance is assessed, i. e. the surface impedance beyond the normal skin effect limit. Parameters which have to be provided for the calculation are the frequency of the HF-wave and the materials parameters charge carrier density, Fermi - velocity and DC-conductivity at the chosen temperature. The CASINOCO - code is set up as a document file of the mathematical software tool MATHCAD.

Berechnung der Oberflächenimpedanz von Normalleitern

Dieser Bericht beschreibt das Programm CASINOCO, mit dem die Oberflächenimpedanz von normalleitenden Materialien bei beliebigen Temperaturen und bei beliebigen Frequenzen bis in den Infrarotbereich berechnet werden können. Dem Programm liegt dabei ein physikalisches Modell zu Grunde, das Beiträge aus nichtlokalen und retardierten Strom-Feld-Korrelationen berücksichtigt und somit die Berechnung des universellen Wertes der Oberflächenimpedanz, d.h. die Berechnung des über den Fall des normalen Skineffekts hinausgehenden Wertes, erlaubt. Parameter, die für die Berechnung zur Verfügung zu stellen sind, umfassen die Frequenz der HF-Welle sowie die Materialparameter Ladungsträgerdichte, Fermi - Geschwindigkeit sowie die Gleichstromleitfähigkeit bei der gewählten Temperatur. Das Programm CASINOCO wurde als eine Dokumentdatei der Mathematik - Software MATHCAD erstellt.

1. Introduction

For the performance of electrically conducting materials in high frequency applications the surface impedance Z (= R + iX) is a key materials parameter. The dissipative term is described by the surface resistance R; the surface reactance X describes the reactive loading and is directly related with the penetration depth λ ($X = \omega\mu\lambda$). An accurate assessment of Z by theoretical models is a non-trivial task when it has to cover the wide frequency and temperature range at which high frequency techniques are presently used.

The classical access to the value of Z is given by the normal skin effect

$$Z = \sqrt{\frac{\omega\mu}{2\sigma}} \cdot (1+i) \qquad (1)$$

where σ is the dc - conductivity of the material , μ its permeability ($\mu = \mu_0\mu_r$) and $\omega = 2\pi f$ the angular frequency of the electromagnetic wave. This analytical expression is a result of the Maxwell equations and Ohm's law and is valid as long as the skin depth δ of the field is much larger than the mean free path l of an electron. At room temperature this assumption is valid for common metals at frequencies up to 100 GHz. For higher frequencies or lower temperatures (equal to higher conductivity) other contributions from the anomalous skin effect and from the Drude relaxation have to be considered. An assessment of Z at general conditions involves the computation of extended integral expressions which can only be solved numerically.

This report describes the formulation of the physical model by the mathematical software tool MATHCAD. With the "CASINOCO" code it is possible to calculate the general value of Z for arbitrary temperatures and frequencies up to the infrared region. Materials parameters which have to be provided for the calculation are the dc - conductivity at the chosen temperature, the electron density and the Fermi-velocity. The underlying physical model [1] was developed by J. Halbritter and will be described briefly in the second chapter. In the third chapter details about the CASINOCO code will be given. The listing of the program is documented in the Appendix.

2. Physical model for the surface impedance

According to the Maxwell equations, the magnetic field is oriented parallel to the surface of planar conductors and Z is given by the penetration of this component $H_{\|}(z, t)$ into the conductor:

$$Z = i\omega\mu \int_0^\infty dz \frac{H_{\|}(z,t)}{H_{\|}(0,t)} = i\omega \frac{A_{\|}(0,t)}{H_{\|}(0,t)} \tag{2}$$

In this notation the z - axis is normal to the surface and directed into the conductor and $A_{\|}$ is the parallel component of the vector potential (rot $\mathbf{A} = \mu\mathbf{H}$). The components $H_{\|}(z, t)$ or $A_{\|}(z, t)$ are the solutions of the following equations and boundary conditions:

- Maxwell equation:

$$-\frac{1}{c^2}\frac{\delta^2 A_{\|}(z,t)}{\delta t^2} + \frac{\delta^2 A_{\|}(z,t)}{\delta z^2} = -j_{\|}(z,t) \tag{3}$$

- material equation (isotropic and homogeneous materials):

$$j_{\|}(z,t) = -\int_{-\infty}^{0} dt' \int dz'\, Q(z-z', t+t')\, A_{\|}(z', t') \tag{4}$$

- boundary conditions for the fields:

$$\left(\frac{A_{\|}(z,t)}{\delta z}\right)_{z=0} = \mu H_{\|}(0,t) \quad ; \quad A_{\|}(\infty, t) = 0 \tag{5}$$

- boundary condition for the charge carriers at the surface:
  specular or diffuse reflection

According to [2] the surface impedance can be written as:

$$Z = i\mu\omega \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dk}{k^2 + \mu Q(k,\omega)} \quad \text{(specular reflection)} \tag{6a}$$

$$Z = i\mu\omega \frac{\pi}{\int_0^\infty dk\, \ln(1 + \mu Q(k,\omega)/k^2)} \quad \text{(diffuse reflection)} \tag{6b}$$

In these equations, Q(k, ω) is the Fourier - transform of the integral kernel Q(z, t) in the material equation (cf. Eq. 3). With the help of the integral kernel Q the material equation

describes the current inside the conductor even in the case of nonlocal and retarded current - field correlation and is therefore the key for a universal description of Z. The integral kernel Q describes the response of the charge carrier system to a photon field and the actual form of $Q(k, \omega)$ is found using quantum field theoretical considerations which are beyond the scope of this report [1,3]:

$$Q(k,\omega) = i\frac{Ne^2}{m}\cdot\hbar\omega\cdot\frac{3}{2}\int_0^{\pi}\frac{\sin\theta\cos\theta d\theta}{\sqrt{\left(\frac{\hbar v_F}{l}+i\omega\right)^2+\left(v_F\hbar k\sin\theta\right)^2}} \tag{7.1}$$

In this expression, N is the electron density of the material, m the electron mass, v_F the Fermi - velocity and l the mean free path.

The physics of the response of a metal to a radio frequency field is generally discussed by the interrelation of three characteristic scales, e.g. the mean free path of an electron l, the flight path of an electron in a 2π - part of a period s and the skin depth of the field δ [2,4,5]. The limits in the relations of these scales define the "pure" cases such as the normal skin effect ($l \ll \delta$, $l \ll s$), anomalous skin effect ($\delta \ll l$, $\delta \ll s$), the relaxation ($s \ll l \ll \delta$), and the anomalous relaxation ($s \ll \delta \ll l$). The characteristic scales can be found also in Eq. 7.1 for $Q(k, \omega)$ and hence in Eq. 6a and 6b for Z, indicating the universal character of the model. Using the definition of the London penetration depth λ_L

$$\lambda_L = \sqrt{\frac{m}{\mu Ne^2}} \tag{8}$$

and the definition of the flight path s

$$s = \frac{v_F}{\omega} \tag{9}$$

Eq. 7.1 can be written as

$$Q(k,\omega) = i\frac{1}{\mu\lambda_L^2}\cdot\frac{3}{2}\int_0^{\pi}\frac{\sin\theta\cos\theta d\theta}{\sqrt{\left(\frac{s}{l}+i\right)^2+(s\,k\sin\theta)^2}} \tag{7.2}$$

showing an explicit dependence of λ_L and the characteristic scales s and l. Further it can be shown that the third characteristic scale δ is also a function of λ_L, s and l:

$$\delta = \lambda_L\sqrt{\frac{s}{l}} \tag{10}$$

For obtaining this equation, the classical definition of δ

$$\delta = \sqrt{\frac{2}{\mu\omega\sigma}} \tag{11}$$

is used where σ is the dc-conductivity. Further, the mean free path l is correlated with the conductivity σ via:

$$l(T) = \frac{mv_F}{Ne^2} \cdot \sigma(T) \tag{12}$$

where the strong temperature dependence of l and σ is indicated. Eq. 10 can be found using Eq. 8,9, 11 and 12.

The procedure to calculate Z for a given material at a selected temperature and frequency is the following: First the parameters l, s and λ_L have to be calculated. This means that the electron density N, the Fermi-velovity v_F and the conductivity σ at the desired temperature have to be known. Using Eq. 7.2, Q (k, ω) can be calculated for each k and then Z can be evaluated by the integrations 6a or 6b in k-space.

In the CASINOCO - code, Z is calculated only for "specular reflection" (cf. Eq. 6a) which was judged to be the more suited case from a physical point of view. Further it was shown in [1] and [4] that there are only minor differences for Z modeled for specular or diffuse reflection. In the pure anomalous skin effect region for example Z exceeds by a factor of 1.125 the value obtained for specular reflection and the difference obviously does not exist in the normal skin effect region. Therefore the exclusive consideration of specular reflection is only a minor restriction of the general validity of CASINOCO.

3. The CASINOCO code: Numerical assessment of the surface impedance

The CASINOCO code is set up as a document file (extension: .MCD) of the commercial mathematical software MATHCAD 6.0 PLUS. This software was chosen for solving the mathematical expressions as it combines the possibility to use a wide variety of built-in functions and routines with the main elements of a modern programming language. In combination with the straight-forward formulation of mathematical expressions, this leads to a very close and transparent program listing which allows a book-like reading. Therefore the following description of CASINOCO's details takes direct reference to the program listing in the Appendix.

CASINOCO is structured in three main sections, e.g. the sections "Input Declarations", "Calculation Routines" and "Performance". Each section reflects the structure in MATHCAD

in which the instructions are successively defined from the left to the right and from the top to the bottom of a document. The main sections will now be described in detail.

Input declarations

The purpose of this section is the declaration of the user-defined input parameters and their conversion into model relevant quantities. In this part the input parameters can be changed according to the material, temperature and frequency set for which the calculations of Z should be carried out.

The listing of this section starts with the definition of the input parameters electron density N, Fermi velocity vF, conductivity σ at temperature T and frequency f. The temperature itself is not needed for the calculation of Z; the setting of this parameter is just for its documentation with the related data set. Further it is possible to adjust the permeability μr of the material, which commonly may be set to $\mu r = 1$ for normal conducting materials used in high frequency applications.

With the help of the declarations for some common constants and definitions, the input parameters are converted to the characteristic scales described in chapter 2, e.g. the London penetration depth λL, the electron's flight path s and the mean free path *lmean*. In addition the skin depth δ is calculated and finally the three characteristic scales δ, s and *lmean* are displayed in units of nanometers for comparison.

Calculation routines

This section contains the definition of all routines necessary to deal with the integrations for evaluating Z. Therefore this section can be called the core of the program.

For the evaluation of Z in specular reflection the integral in Eq. 6a has to be carried out over the whole k-axis. For this purpose the integral kernel Q (k, ω) (cf. chapter 2) is determined for each value of k which involves the computation of the integral in Eq. 7.2 over the finite angle interval from 0 to π. Therefore, to evaluate Z one has to deal with two encapsulated integrations. This problem is solved by the possibility to program user-defined functions in MATHCAD which can be used like any built-in function.

The program listing of this section starts with the definition of the routine for calculating the integral kernel Q(k, ω). It is composed of the definition of the function 'QTeil' and the definition of the subroutine 'Q'. The function 'QTeil' is defined corresponding to the integral in Eq. 7.2. but with a variable and adjustable interval from a to b. It is used in the subroutine 'Q', where the integration over the finit angle interval from 0 to π (cf. Eq. 7.2) is cut in *nmax* parts.

This is necessary to ensure a proper calculation of the integral kernel in the relevant k-space. The integration is carried out over each part and the results are added. The final result of the subroutine 'Q' is a complex number which is except for a factor identical to the integral kernel for specified *k*, *l* and *s*.

The rest of this section is devoted to the integration in k-space (cf. Eq. 6a). First, the strategy of this integration has to be outlined. By symmetry arguments the integration over the whole k-axis is reduced to the double value of the integration over the half axis from 0 to infinity. The integration is carried out by successive steps along the positive k-axis and the results are added. In order to deal numerically with the integration towards infinity a cut-off condition is created to terminate the calculation based on the fact, that there are no problems of convergence of this integral in a mathematical sense. The cut-off occurs if the additive term from the last integration is smaller than a specified limit.

The listing of the routine for the k-integration is composed of the definitions of the function 'Int', the subroutine 'Framepara' and the subroutine 'Integral'. The function 'Int' is declared as an integral corresponding to Eq. 6a but again with a adjustable integration range. Further a scaling factor 10^{15} is introduced to deal with sufficiently large numbers for the integration routine of MATHCAD.

The subroutine 'Framepara' determines the frame parameters of the successive integration steps along the k-axis, e.g. the length, the upper and the lower border of the integration interval and the limit of the cut-off condition. The result of this subroutine is a four-dimensional vector with the following components:

v_1: lower border of the integration interval
v_2: upper border of the integration interval
v_3: length of the interval
v_4: limit of the cut-off condition

Detailed information about the length of the intervals along the k-axis are given beneath the listing of the subroutine 'Framepara' in the Appendix. Further it should be mentioned that the accuracy of the calculation of Z can be influenced by changing the parameter *limit* in this subroutine. The exact meaning of this parameter is explained in the following description of the subroutine 'Integral'.

In the subroutine 'Integral' finally the execution of the integration of Eq. 6a is defined using directly or indirectly all the definitions above. It is this subroutine which will be used directly in the section "Performance" to carry out the calculation of Z.

Starting with a first integration in the interval $k = 0$ to $k = 10^6$ the computation proceeds inside a loop when it carries out the integration by successive steps given by the subroutine 'Framepara' and adds up the results. The variables *NewVal* and *OldVal* contain successively the actual and the previous result of the integration steps. The loop ends if the difference between the variables *NewVal* and *OldVal* is smaller than the specified parameter *limit* in both, the real part and the imaginary part. The result of the subroutine "Integral" is the surface impedance for the parameters l, s, ω and μr from the general model.

The unit of the result is [mΩ] and this is therefore also the unit of the variables *NewVal, OldVal* and the parameter *limit*, specified in the subroutine 'Framepara'. The parameter *limit* is an upper limit for the increase of the latest result due to the next integration step. In this way the accuracy of the calculation is influenced by the parameter *limit*.

Performance

The role of this code section is to start the calculation of Z and to display the result. The calculation is initialized by the declaration of the variable *Zsurface* using the subroutine 'Integral'. The parameter list of the subroutine contains the parameters *lmean*, s, ω and μr, declared in the section "Input-Declarations". The calculation starts when rolling down the document to the declaration of *Zsurface*. The result of the calculation is displayed in the next line together with the temperature and the frequency set in the section "Input Declaration".

The calculation of *Zsurface* takes some time, normally 20 to 120 minutes depending on the input parameters and the computer performance. It is possible to stop the execution by pressing the key "Esc". The execution can be restarted by clicking on the declaration of *Zsurface* and pressing the function key "F9".

The listing of the program CASINOCO is terminated by the calculation of Z for the special cases 'normal skin effect' and 'anomalous skin effect'. The results are displayed also in milliohm to be compared with the result of the universal model.

4. References

[1] J. Halbritter; unpublished report

[2] J. Halbritter; Externer Bericht 3/69-2; Kernforschungszentrum Karlsruhe 1969

[3] A. A. Abrikosov, L. P. Gorkov, I. Yu. Dzyaloshskii; Quantum Field Theoretical Methods in Statistical Physics, Pergamon Press, N. Y. 1965

[4] G. E. H. Reuter, E. H. Sondheimer; Proc. Roy. Soc. A 195, 336 (1948)

[5] H. B. G. Casimir, J. Ubbink; Philips Technische Rundschau 28, 204 (1967)

Appendix: Program Listing

Program CASINOCO:
Calculation of the Surface Impedance of Normal Conductors
at arbitrary frequencies and temperatures

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Date: 09.08.1996

INPUT - DECLARATIONS

Input parameters:

$N := 8.45 \cdot 10^{28}$ **electron density [1/m^3]**

$vF := 1.7 \cdot 10^{6}$ **Fermi - velocity [m/s]**

$\sigma := 5.796 \cdot 10^{7}$ **conductivity [1/(Ωm)]**

$T := 300$ **temperature [K]**

$f := 145 \cdot 10^{9}$ **frequency for which calculation should be done [Hz]:**

$\mu r := 1$ **permeability**

Declarations of common constants and definitions

$\mu 0 := 4 \cdot \pi \cdot 10^{-7}$

$\omega := 2 \cdot \pi \cdot f$

$me := 9.1095 \cdot 10^{-31}$

$\mu := \mu r \cdot \mu 0$

$e := 1.60219 \cdot 10^{-19}$

$TOL := 10^{-10}$ **internal parameter of MATHCAD**

Calculation of the parameters λ_L , s(ω), l(T) using the data above

$\lambda L := \sqrt{\frac{me}{\mu \cdot N \cdot e^2}}$ **London penetration depth [m]**

$s := \frac{vF}{\omega}$ **flight distance of an electron in 1/2π - part of a periode [m]**

$lmean := \frac{me \cdot vF \cdot \sigma}{N \cdot e^2}$ **mean free path of an electron [m]**

Additional parameters (not necessary for calculation):

$\delta sk := \sqrt{\frac{2}{\omega \cdot \mu \cdot \sigma}} \cdot 10^9$ **skin depth [nm]**

$lnm := lmean \cdot 10^9$ **mean free path [nm]**

$snm := s \cdot 10^9$ **flight distance [nm]**

T [K]	l(T) [nm]	δ(T,ω) [nm]	s(ω) [nm]
$T = 300$	$lnm = 41.38$	$\delta sk = 173.609$	$snm = 1.866 \cdot 10^3$

CALCULATION ROUTINES

Routine for the calculation the intergral - kernel Q(k,ω)

Function QTeil:

$$QTeil(k,l,s,a,b) := \frac{3i}{2} \cdot \int_a^b \frac{\sin(\theta)\cdot\cos(\theta)^2}{\sqrt{\left(\frac{s}{l}+i\right)^2 + (s\cdot k\cdot\sin(\theta))^2}}\, d\theta$$

Subroutine Q: Angle - integration from θ = 0 to π

$Q(k,l,s) :=$
- Summe ← 0
- nmax ← 30
- for $n \in 1..nmax$
  - $a \leftarrow (n-1)\cdot\frac{\pi}{nmax}$
  - $b \leftarrow n\cdot\frac{\pi}{nmax}$
  - Summe ← Summe + QTeil(k,l,s,a,b)
- Summe

Declarations of the routines for the k - space integration

Function Int:

$$fsp(k,l,s) := \frac{1\cdot 10^{15}}{k^2 + \frac{1}{\lambda L^2}\cdot Q(k,l,s)} \qquad Int(a,b,l,s) := \int_a^b fsp(k,l,s)\, dk$$

Subroutine Framepara: Setting the frame parameters of the integration in k - space

Frame parameters are

- **length, lower and upper border of the integration interval**
- **parameter for the cut-off condition**

```
Framepara(a, b, step) := | if b < 10^9
                         |     step ← 10·step
                         |     aold ← a
                         |     a ← b
                         |     b ← 10·step
                         |     limit ← 0.05
                         | otherwise
                         |     step ← 10^8
                         |     aold ← a
                         |     a ← b
                         |     b ← b + step
                         |     limit ← 0.05
                         | v_0 ← a
                         | v_1 ← b
                         | v_2 ← step
                         | v_3 ← limit
                         | v
```

Information about the actual settings:

Below k = 10^9 the next integration step will be increased by a factor of 10

Below k = 10^9 the calculation will be stopped if the difference between two sucessive steps will be smaller then *limit* [mΩ]

Above k = 10^9 the next interation step will be increased by adding *step*

Above k = 10^9 the calculation will be stopped if the difference between two sucessive steps will be smaller then *limit* [mΩ]

Subroutine Integral: Carrying out the calculating the surface impedance

$$\text{Integral}(l, s, \omega, \mu r) :=$$

$\text{OldVal} \leftarrow 0$

$\text{step} \leftarrow 10^5$

$a \leftarrow 10^5$

$b \leftarrow 10^6$

$\text{limit} \leftarrow 0$

$v_0 \leftarrow a$

$v_1 \leftarrow b$

$v_2 \leftarrow \text{step}$

$v_3 \leftarrow \text{limit}$

$\text{NewVal} \leftarrow i \cdot \mu r \cdot 8 \cdot \omega \cdot 10^{-19} \cdot \text{Int}(0, 10^6, 1, s)$

$\text{bool1} \leftarrow |\text{Re}(\text{NewVal}) - \text{Re}(\text{OldVal})| > \text{limit}$

$\text{bool2} \leftarrow |\text{Im}(\text{NewVal}) - \text{Im}(\text{OldVal})| > \text{limit}$

while bool1 + bool2

- $w \leftarrow \text{Framepara}(v_0, v_1, v_2)$
- $v \leftarrow w$
- $\text{OldVal} \leftarrow \text{NewVal}$
- $\text{NewVal} \leftarrow \text{NewVal} + i \cdot \mu r \cdot 8 \cdot \omega \cdot 10^{-19} \cdot \text{Int}(w_0, w_1, 1, s)$
- $\text{bool1} \leftarrow |\text{Re}(\text{NewVal}) - \text{Re}(\text{OldVal})| > w_3$
- $\text{bool2} \leftarrow |\text{Im}(\text{NewVal}) - \text{Im}(\text{OldVal})| > w_3$

$\text{IntegVal} \leftarrow \text{NewVal}$

IntegVal

PERFORMANCE

Start of the programm and documentation of the result:

Zsurface := Integral (lmean,s,ω,μr)

Zsurface = 97.71139 + 100.96845i **at** T = 300K and f = 145 GHz

In addition:
Surface impedance for the pure cases of the normal and anomalous skin effect

normal skin effect:

$$Zs := 10^3 \cdot \omega \cdot \mu \cdot \lambda L \cdot \sqrt{\frac{s}{2 \cdot lmean}} \cdot (1 + i)$$

$Zs = 99.38 + 99.38i$ **mΩ.**

anomalous skin effect (temperature independent):

$$Zs := 10^3 \cdot \omega \cdot \mu \cdot \frac{\lambda L}{9} \cdot 4 \cdot \left(\frac{\sqrt{3} \cdot s}{2 \cdot \pi \cdot \lambda L} \right)^{\frac{1}{3}} \cdot \left(1 + \sqrt{3} \cdot i \right)$$

$Zs = 28.292 + 49.004i$ **mΩ**